

09/763,740

=> d his

(FILE 'HOME' ENTERED AT 12:46:36 ON 01 MAY 2002)

FILE 'REGISTRY' ENTERED AT 12:47:08 ON 01 MAY 2002

L1 STRUCTURE UPLOADED  
L2 1 S L1  
L3 22 S L1 FUL

FILE 'REGISTRY' ENTERED AT 12:48:04 ON 01 MAY 2002

L4 1 S L3

FILE 'CAPLUS' ENTERED AT 12:48:15 ON 01 MAY 2002

L5 1 S L3

=> d l1

L1 HAS NO ANSWERS

L1 STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

=> d bib abs hitstr l5

L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS

AN 1998:65889 CAPLUS

DN 128:127826

TI Preparation of new amidino derivatives as thrombin inhibitors

IN Antonsson, Thomas

PA Astra Aktiebolag, Swed.; Antonsson, Thomas

SO PCT Int. Appl., 108 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9801422	A1	19980115	WO 1997-SE1150	19970626
	W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
	CA 2260190	AA	19980115	CA 1997-2260190	19970626
	AU 9735628	A1	19980202	AU 1997-35628	19970626
	AU 726236	B2	20001102		
	EP 917528	A1	19990526	EP 1997-932085	19970626
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
	BR 9710142	A	19990810	BR 1997-10142	19970626
	CN 1228765	A	19990915	CN 1997-197578	19970626
	JP 2000515505	T2	20001121	JP 1998-505123	19970626
	US 6221898	B1	20010424	US 1997-894833	19970829
	NO 9806180	A	19990304	NO 1998-6180	19981229
	KR 2000022437	A	20000425	KR 1998-710870	19981230
	US 2002040043	A1	20020404	US 2001-839609	20010423
PRAI	SE 1996-2646	A	19960704		

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WO 1997-SE1150 W 19970626  
US 1997-894833 A3 19970829  
OS MARPAT 128:127826  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

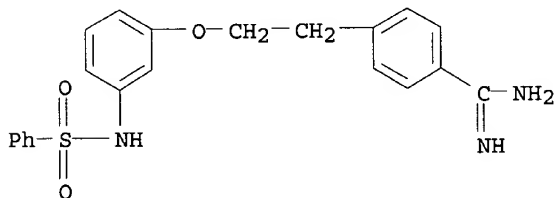
AB The title compds. [I; one of R1 and R2 = Z-SO<sub>2</sub>-Ar1 and the other = R4; Z = O, NR<sub>5</sub>; R3 = Oh, halo, Cn, etc.; R4 = H, OH, halo, etc.; Ar1 = Ph, C1-3 alkylphenyl, naphthyl, etc.; R5 = H, C1-6 alkyl, Ph, C1-3 alkylphenyl; Y = O, S, S(O), SS(O)<sub>2</sub>, NR<sub>22</sub>; R22 = H, C1-4 alkyl; n = 0-4; B = II, III, IV, V; X1, X2 = a single bond, CH<sub>2</sub>], useful as competitive inhibitors of trypsin-like proteases, such as thrombin, and in particular in the treatment of conditions where inhibition of thrombin is required (e.g. thrombosis) or as anticoagulants, were prepd. Thus, reaction of 3-[2-(4-cyanophenyl)ethoxy]aniline with benzenesulfonyl chloride followed by treatment of the resulting N-{3-[2-(4-cyanophenyl)ethoxy]phenyl}benzenesulfonamide with HCl(g) in EtOH, and treating N-{3-[2-(4-ethoxyiminomethylphenyl)ethoxy]phenyl}benzenesulfonamide.HCl with NH<sub>3</sub>(g) afforded the title compd. VI. The title compds. I described herein were tested for thrombin inhibition and were found to exhibit an IC<sub>50</sub> and/or Ki (as appropriate) of < 0.3 .mu.M.

IT 201933-65-5P 201933-67-7P 201933-68-8P  
201933-69-9P 201933-70-2P 201933-71-3P  
201933-72-4P 201933-73-5P 201933-80-4P  
201933-81-5P 201933-82-6P 201933-83-7P  
201933-84-8P 201933-85-9P 201934-61-4P  
201934-62-5P 201934-63-6P 201934-64-7P  
201934-65-8P 201934-71-6P 201934-72-7P  
201935-44-6P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of new amidino derivs. as thrombin inhibitors)

RN 201933-65-5 CAPLUS

CN Benzenecarboximidamide, 4-[2-[3-[(phenylsulfonyl)amino]phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

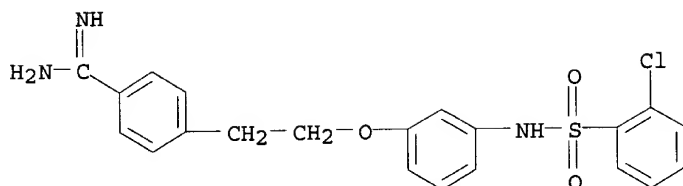


● HCl

RN 201933-67-7 CAPLUS

CN Benzenecarboximidamide, 4-[2-[3-[[2-chlorophenyl)sulfonyl]amino]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

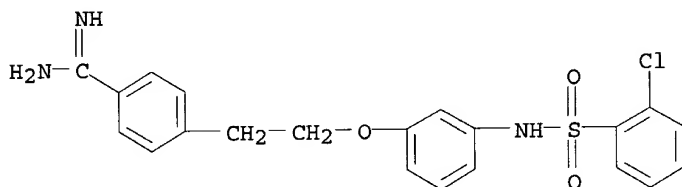
09/763,740



RN 201933-68-8 CAPLUS  
CN Benzenecarboximidamide, 4-[2-[3-[[2-chlorophenyl)sulfonyl]amino]phenoxy]ethyl]-, monoacetate (9CI) (CA INDEX NAME)

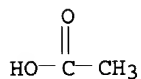
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CRN 201933-67-7  
CMF C21 H20 Cl N3 O3 S

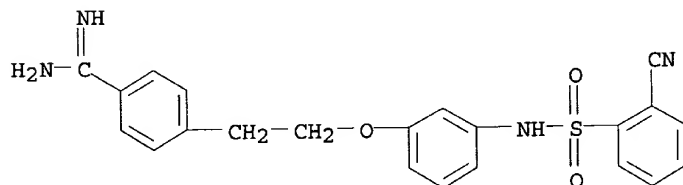


CM 2

CRN 64-19-7  
CMF C2 H4 O2



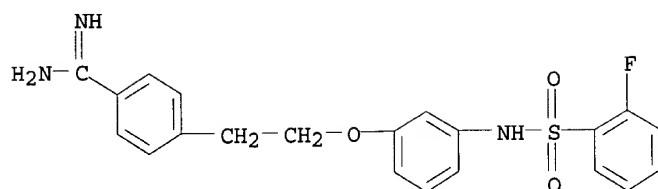
RN 201933-69-9 CAPLUS  
CN Benzenecarboximidamide, 4-[2-[3-[[2-cyanophenyl)sulfonyl]amino]phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

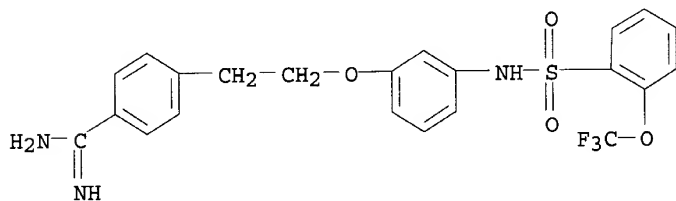
RN 201933-70-2 CAPLUS  
CN Benzenecarboximidamide, 4-[2-[3-[[2-fluorophenyl)sulfonyl]amino]phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

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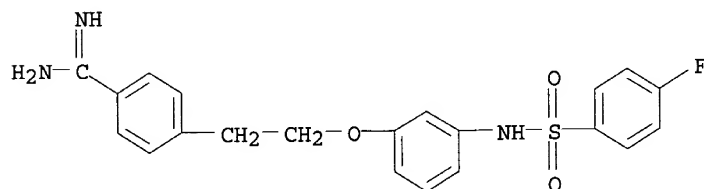
● HCl

RN 201933-71-3 CAPLUS  
CN Benzenecarboximidamide, 4-[2-[3-[[[2-(trifluoromethoxy)phenyl]sulfonyl]amino]phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

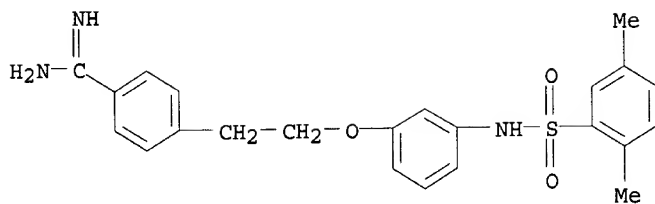
RN 201933-72-4 CAPLUS  
CN Benzenecarboximidamide, 4-[2-[3-[[[2-(trifluoromethoxy)phenyl]sulfonyl]amino]phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

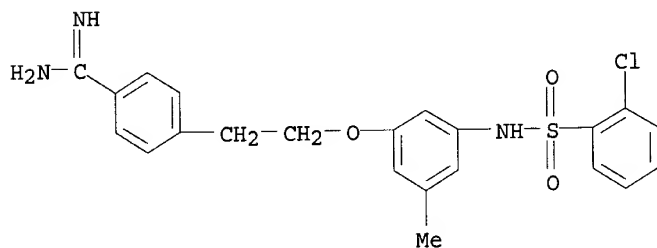
RN 201933-73-5 CAPLUS  
CN Benzenecarboximidamide, 4-[2-[3-[[[2-(trifluoromethoxy)phenyl]sulfonyl]amino]phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

09/763,740



● HCl

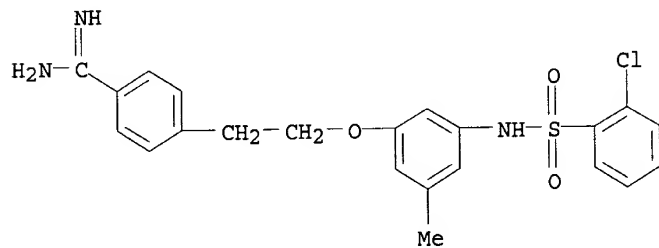
RN 201933-80-4 CAPLUS  
CN Benzenecarboximidamide, 4-[2-[3-[[[2-(4-methylphenyl)sulfonyl]amino]-5-methylphenoxy]ethyl]- (9CI) (CA INDEX NAME)



RN 201933-81-5 CAPLUS  
CN Benzenecarboximidamide, 4-[2-[3-[[[2-(2-chlorophenyl)sulfonyl]amino]-5-methylphenoxy]ethyl]-, monoacetate (9CI) (CA INDEX NAME)

CM 1

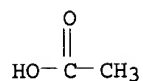
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CMF C22 H22 Cl N3 O3 S



CM 2

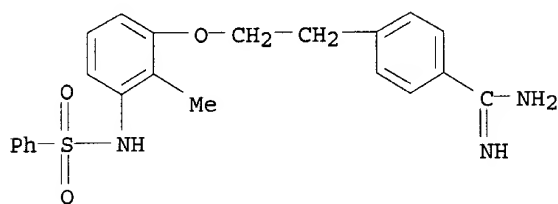
CRN 64-19-7  
CMF C2 H4 O2

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RN 201933-82-6 CAPLUS

CN Benzenecarboximidamide, 4-[2-[2-methyl-3-[(phenylsulfonyl)amino]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



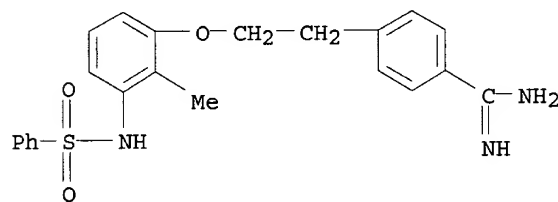
RN 201933-83-7 CAPLUS

CN Benzenecarboximidamide, 4-[2-[2-methyl-3-[(phenylsulfonyl)amino]phenoxy]ethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 201933-82-6

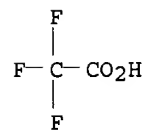
CMF C22 H23 N3 O3 S



CM 2

CRN 76-05-1

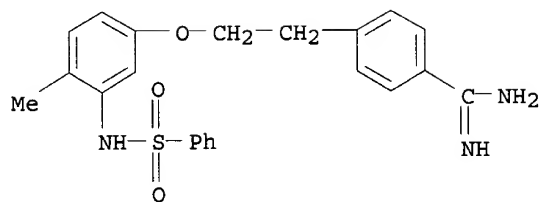
CMF C2 H F3 O2



RN 201933-84-8 CAPLUS

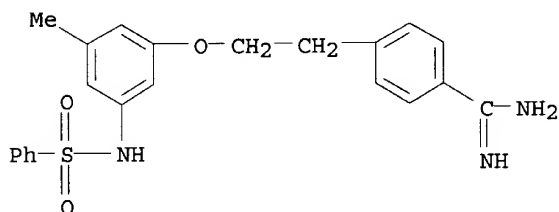
CN Benzenecarboximidamide, 4-[2-[4-methyl-3-[(phenylsulfonyl)amino]phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

09/763,740



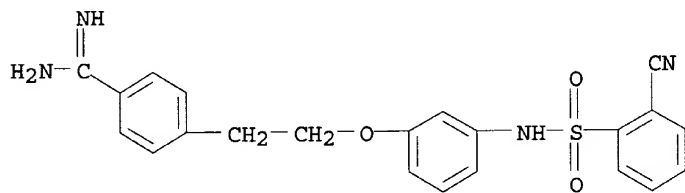
● HCl

RN 201933-85-9 CAPLUS  
CN Benzenecarboximidamide, 4-[2-[3-methyl-5-[(phenylsulfonyl)amino]phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

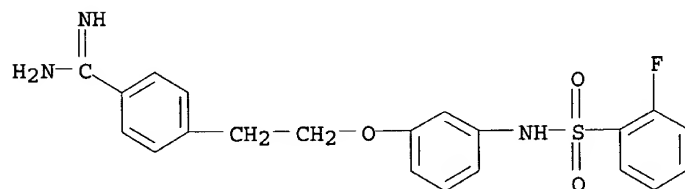


● HCl

RN 201934-61-4 CAPLUS  
CN Benzenecarboximidamide, 4-[2-[3-[[2-(cyanophenyl)sulfonyl]amino]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



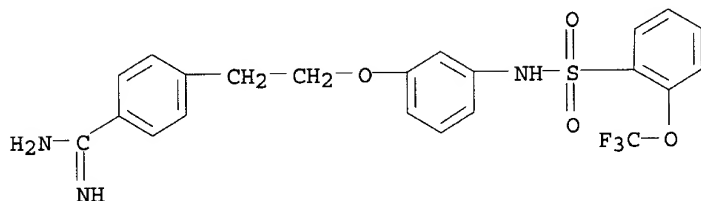
RN 201934-62-5 CAPLUS  
CN Benzenecarboximidamide, 4-[2-[3-[[2-(fluorophenyl)sulfonyl]amino]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



RN 201934-63-6 CAPLUS

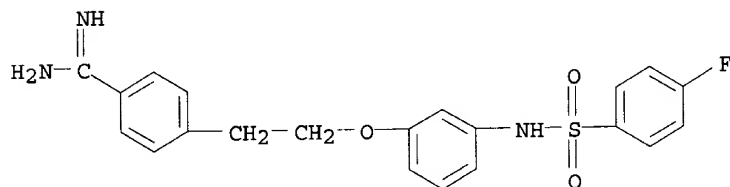
09/763,740

CN Benzenecarboximidamide, 4-[2-[3-[[[2-(trifluoromethoxy)phenyl]sulfonyl]amino]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



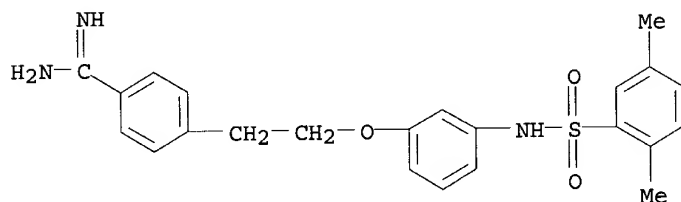
RN 201934-64-7 CAPLUS

CN Benzenecarboximidamide, 4-[2-[3-[[[4-fluorophenyl]sulfonyl]amino]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



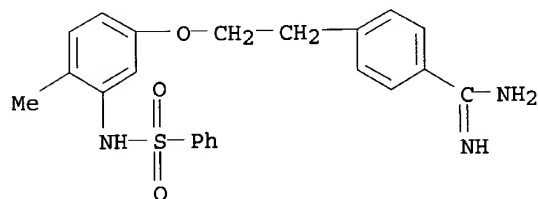
RN 201934-65-8 CAPLUS

CN Benzenecarboximidamide, 4-[2-[3-[[[2,5-dimethylphenyl]sulfonyl]amino]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



RN 201934-71-6 CAPLUS

CN Benzenecarboximidamide, 4-[2-[4-methyl-3-[(phenylsulfonyl)amino]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

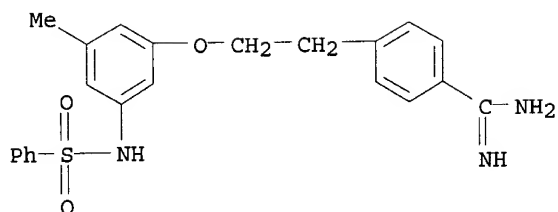


RN 201934-72-7 CAPLUS

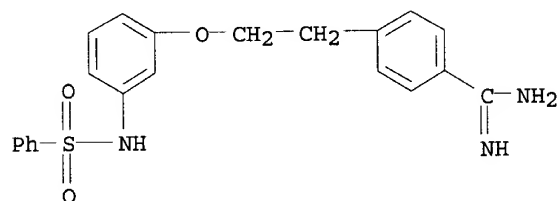
CN Benzenecarboximidamide, 4-[2-[3-methyl-5-[(phenylsulfonyl)amino]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



09/763,740

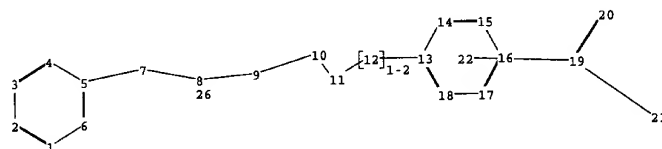
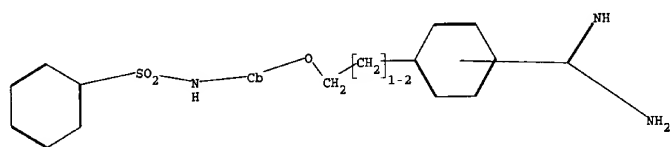


RN 201935-44-6 CAPLUS  
CN Benzenecarboximidamide, 4-[2-[3-[(phenylsulfonyl)amino]phenoxy]ethyl]-  
(9CI) (CA INDEX NAME)



=>

C:\STNEXP4\QUERIES\839.str



chain nodes :

7 8 9 10 11 12 19 20 21 26

ring nodes :

1 2 3 4 5 6 13 14 15 16 17 18

chain bonds :

5-7 7-8 8-9 8-26 9-10 10-11 11-12 12-13 19-20 19-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds :

7-8 19-20 19-21

exact bonds :

5-7 8-9 8-26 9-10 10-11 11-12 12-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS  
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS  
20:CLASS 21:CLASS 22:CLASS 26:CLASS

Generic attributes :

9:

Saturation : Unsaturated  
Number of Carbon Atoms : less than 7  
Type of Ring System : Monocyclic

Element Count :

Node 9: Limited  
C,C6